L7 L8 L9 L10	FILE	'REGISTRY' ENTERED AT 13:22:47 ON 31 JUL 2008 STRUCTURE UPLOADED STRUCTURE UPLOADED STRUCTURE UPLOADED STRUCTURE UPLOADED
L11		1 S L10
L12		22 S L10 SSS FULL
L13	FILE	'CAPLUS' ENTERED AT 13:52:40 ON 31 JUL 2008 5 S L12
	FILE	'REGISTRY' ENTERED AT 14:02:04 ON 31 JUL 2008
L14		STRUCTURE UPLOADED
L15		0 S L14
L16		0 S L14 SSS FULL

### PASSWORD:

\* \* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \* SESSION RESUMED IN FILE 'REGISTRY' AT 13:51:21 ON 31 JUL 2008 FILE 'REGISTRY' ENTERED AT 13:51:21 ON 31 JUL 2008 COPYRIGHT (C) 2008 American Chemical Society (ACS)

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 2.30 213.12 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE 0.00 -8.00

Uploading C:\Program Files\STNEXP\Queries\10780447linker.str

chain nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44

45 46

chain bonds : 1-2 1-3 1-4 2-5 3-6 4-7 5-14 6-11 7-8 8-9 9-10 10-19 10-20 11-12 12-13

13-18 13-21 14-15 15-16 16-17 16-22 17-23 17-45 18-25 18-46 19-27 19-41 23-24 24-31

25-26 26-30 27-28 28-29 29-34 29-42 30-33 30-43 31-32 31-44 32-37 32-40

33-36 33-39 34-35 34-38

exact/norm bonds : 10-19 10-20 13-18 13-21 16-17 16-22 29-34 30-33 31-32 32-37 33-36 34-35

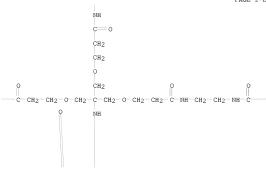
exact bonds :

 $1-2 \quad 1-3 \quad 1-4 \quad 2-5 \quad 3-6 \quad 4-7 \quad 5-14 \quad 6-11 \quad 7-8 \quad 8-9 \quad 9-10 \quad 11-12 \quad 12-13 \quad 14-15 \quad 15-16$ 17-23 17-45 18-25 18-46 19-27 19-41 23-24 24-31 25-26 26-30 27-28 28-29

29-42 30-43 31-44 32-40 33-39 34-38

```
Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS
18:CLASS 19:CLASS
20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS
28:CLASS 29:CLASS
30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS
38:CLASS 39:CLASS
40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS
T-10
       STRUCTURE UPLOADED
=> 8 110
SAMPLE SEARCH INITIATED 13:51:46 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -
                                   901 TO ITERATE
100.0% PROCESSED
                    901 ITERATIONS
                                                              1 ANSWERS
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                             **COMPLETE**
                       BATCH
PROJECTED ITERATIONS:
                           16220 TO
                                      19820
PROJECTED ANSWERS:
                               1 TO
                                          80
             1 SEA SSS SAM L10
=> d 111 scan
L11 1 ANSWERS
               REGISTRY COPYRIGHT 2008 ACS on STN
    Gadolinium, aqua[6,9-bis[(carboxy-\kappa0)methyl]-21-[(4-0-\beta-D-
TN
    galactopyranosyl-D-gluconoyl)amino]-3-[2-[[2-[3-[[2-[(4-0-β-D-
    galactopyranosyl-D-gluconoyl)amino]ethyl]amino]-3-oxopropoxy]-1,1-bis[[3-
    [[2-[(4-O-β-D-galactopyranosyl-D-gluconoyl)amino]ethyl]amino]-3-
    [3-[2-(4-\cos^2\theta)]
    O-β-D-galactopyranosyl-D-gluconoyl)amino]ethyl]amino]-3-
    oxopropoxy]methyl]-11-(oxo-<math>\kappa O)-18-oxo-15-oxa-3,6,9,12,19-
    pentaazaheneicosanoato(3-)-KN3, KN6, KN9, KO1]-
    C124 H220 Gd N17 087
MF
CI
    CCS
```

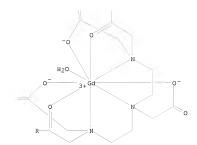
## PAGE 2-A



PAGE 2-C

0==

PAGE 3-B



PAGE 4-A

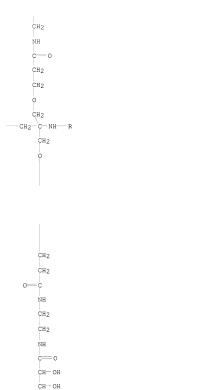
НО---

но\_\_

но-сн2-

PAGE 5-A

PAGE 6-B



HO-

PAGE 7-B

22 ANSWERS

#### ALL ANSWERS HAVE BEEN SCANNED

#### => 0

#### 0 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

## => 0

#### 0 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (->).

# => s 110 sss full

FULL SEARCH INITIATED 13:52:35 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 17973 TO ITERATE

100.0% PROCESSED 17973 ITERATIONS SEARCH TIME: 00.00.01

SEARCH TIME: UU.UU.UI

L12 22 SEA SSS FUL L10

=> file caplus

 COST IN U.S. DOLLARS
 SINCE FILE
 TOTAL

 ENTRY
 SESSION

 FULL ESTIMATED COST
 181.12
 391.94

TOTAL. SESSION ENTRY 0.00 -8.00

CA SUBSCRIBER PRICE

FILE 'CAPLUS' ENTERED AT 13:52:40 ON 31 JUL 2008 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 31 Jul 2008 VOL 149 ISS 5 FILE LAST UPDATED: 30 Jul 2008 (20080730/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/legal/infopolicy.html

=> s 112 L13

AB

5 L12

=> d 113 1-5 ti abs bib hitstr

- L13 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
- Preparation of monosaccharide- and oligosaccharide-containing gadolinium ΤI compounds and contrast medium for MRI
- \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT \*
- Gadolinium compds, represented by the following general formula (I) [R = (G1-NHCH2CH2)2N, [(G2-NHCH2CH2)2NCOCH2CH2OCH2]3C; G1 or G2 represents a residue formed by reacting a sugar lactone with an amino group, the sugar of the sugar lactone representing allose, altrose, mannose, gulose, idose, galactose, talose, ribose, arabinose, xylose, lyxose, erythrose, threose, cellobiose, maltose, lactose, or maltotriose], are prepared The novel gadolinium compds. (1) have a high spin-lattice relaxation (T1) property and can form an image with high sensitivity even when administered in a small amount, (2) are highly effective in imaging systemic blood vessels and the liver, (3) are highly effective in imaging the pancreas, and (4) have such safety that most of the compound is discharged from the body within 24 h. There is also provided a MRI contrast medium containing the compound I. Thus, ring-opening amidation of allonolactone with diethylenetriamine in DMF at room temperature followed by N-protection with di(tert-butyl)

dicarbonate

```
in DMF, acetylation of the sugar moiety with acetic anhydride in pyridine,
     and removing the Boc group with CF3CO2H in CH2C12 at room temperature gave the
     amide (O3-H; R1 = Ac) which underwent amidation with 2-[N,N-bis[2-(2,6-
     dioxomorpholin-4-yl)ethyl]amino]acetic acid (DTPA dianhydride) in DMF to
     give the amide (II; R1 = Ac). II was heated with Gd203 in H20 at
     100° followed by treatment with 1 M aqueous NaOH solution at 40° to
     give allonamide-containing DTPA-gadolinium complex I (R = Q3; R1 = H) which
     showed 1/T1 of 40.5 s-1.
     2008:473521 CAPLUS <<LOGINID::20080731>>
     148:485896
     Preparation of monosaccharide- and oligosaccharide-containing gadolinium
     compounds and contrast medium for MRI
     Miura, Norio; Yamashita, Mitsuji
     National University Corporation Shizuoka University, Japan; Konica Minolta
     Holdings, Inc.
     PCT Int. Appl., 121pp.
     CODEN: PIXXD2
     Patent
     Japanese
FAN.CNT 1
     PATENT NO.
                         KIND
                                 DATE
                                             APPLICATION NO.
                                                                     DATE
                         ____
                                                                     20070920
     WO 2008044443
                          A1
                                 20080417
                                            WO 2007-JP68298
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA,
             CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG,
             KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME,
             MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL,
             PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN,
             TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF,
             BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW,
             GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
             BY, KG, KZ, MD, RU, TJ, TM
PRAI JP 2006-274710
                          A
                                 20061006
   MARPAT 148:485896
     1020112-53-1P 1020112-54-2P 1020112-55-3P
     1020112-56-4P 1020213-18-6P 1020213-19-7P
     1020213-20-0P 1020213-21-1P 1020213-22-2P
     1020213-23-3P 1020213-24-4P 1020213-25-5P
     1020213-26-6P 1020213-27-7P 1020213-29-9P
     1020213-30-2P
     RL: BSU (Biological study, unclassified); DGN (Diagnostic use); PRP
     (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP
     (Preparation); USES (Uses)
        (preparation of monosaccharide- and oligosaccharide-containing gadolinium
DTPA
        compds. and contrast media containing them for MRI)
     1020112-53-1 CAPLUS
     Gadolinium, [21-(D-allonoylamino)-3-[2-[[2-[3-[[2-(D-
     allonoylamino)ethyl]amino]-3-oxopropoxy]-1,1-bis[[3-[[2-(D-
     allonovlamino)ethyllaminol-3-oxopropoxylmethyllethyllaminol-2-(oxo-
     κO) ethyl]-13, 13-bis[[3-[[2-(D-allonoylamino)ethyl]amino]-3-
     oxopropoxy]methyl]-11-(oxo-\kappa0)-18-oxo-15-oxa-3,6,9,12,19-
     pentaazaheneicosanoato(3-)-KN3, KN6, KN9, KO1]aqua-
     (CA INDEX NAME)
```

AN

DN

ΤI

IN

PA

SO

DT

LA

ΡI

OS

IT

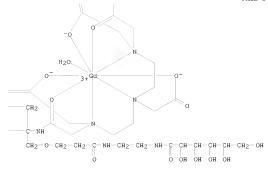
RN

CN

PAGE 1-B

$$-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{NH}-\mathsf{C}-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{O}-\mathsf{CH}_2\\ \mathsf{NH}-\mathsf{C}-\mathsf{CH}_2-\mathsf{O}-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{C}-\mathsf{NH}-\mathsf{CH}_2-\mathsf{CH}_2\\ \mathsf{CH}_2-\mathsf{O}-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{C}-\mathsf{NH}-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{NH}-\\ \mathsf{O} \\ \mathsf{O}$$

PAGE 2-A

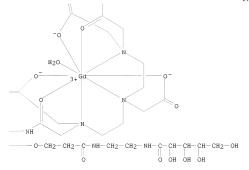


- RN 1020112-54-2 CAPLUS
- CN Gadolinium, aqua[6,9-bis[(carboxy-KO)methyl]-11-(oxo-KO)-18oxo-3-[2-(oxo-KO)-2-[[2-[3-oxo-3-[(2-(Dribonoylamino)ethyl]amino]propxy]-1,1-bis[[3-oxo-3-[[2-(Dribonoylamino)ethyl]amino]propxy]methyl]pethyl]amino]ethyl]-13,13-bis[[3oxo-3-[[2-(D-ribonoylamino)ethyl]amino]propxy]methyl]-21-(Dribonoylamino)-15-oxa-3,6,9,12,19-pentaazaheneicosanoato(3-)kN3,KN,KN9,KO]-(CA INDEX NAME)

PAGE 1-A

PAGE 1-C

PAGE 2-B



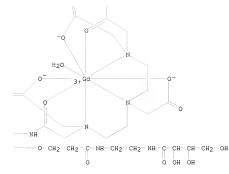
RN 1020112-55-3 CAPLUS CN Gadolinium, aqua[24.

 $\begin{array}{lll} {\rm Gadolinium,\ aqua[24,25,26-trihydroxy-11-(oxo-κ0)-18,23-dioxo-3-[15,16,17-trihydroxy-2-(oxo-κ0)-9,14-dioxo-13,13-bis[[3-oxo-3-[12-[(2,3,4-trihydroxy-1-oxobuty1)amino]ethyl]amino]propoxy]methyl]-4,4-bis[[3-oxo-3-[[2-[(2,3,4-trihydroxy-1-oxobuty1)amino]ethyl]amino]propoxy]methyl]-6-oxa-3,10,13-triazaheptadec-1-yl]-15-oxa-3,6,9,12,19,22-hexaa:ahexacosanoato(3-)-κN3,κN6,κN9,κO1]- (CA$ 

PAGE 1-B

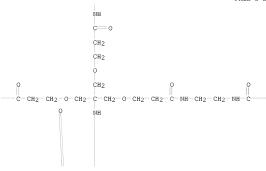
$$\begin{array}{c} -- \operatorname{ch}_2 - \operatorname{nh} - \operatorname{C} - \operatorname{ch}_2 - \operatorname{ch}_2 - \operatorname{o} - \operatorname{ch}_2 \\ -- \operatorname{nh} - \operatorname{c} - \operatorname{ch}_2 - \operatorname{ch}_2 - \operatorname{c} - \operatorname{ch}_2 - \operatorname{ch}_2$$

PAGE 2-A



- RN 1020112-56-4 CAPLUS
- NN 1020112-06-4 CAPLOS CAPL

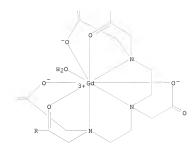
## PAGE 2-A



PAGE 2-C

0==

PAGE 3-B



PAGE 4-A

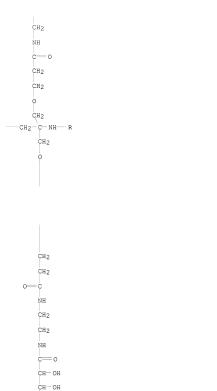
НО---

но\_\_

но-сн2-

PAGE 5-A

PAGE 6-B



но

PAGE 7-B

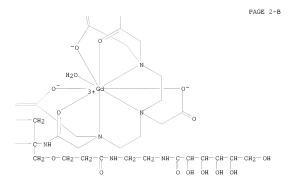
RN 1020213-18-6 CAPLUS

CN Gadolinium, [2]-[D-altronoylamino]-3-[2-[2-[3-[2-(D-altronoylamino) ethyl]amino]-3-oxopropoxy]-1,1-bis[[3-[2-(D-altronoylamino) ethyl]amino]-3-oxopropoxy]methyl]ethyl]amino]-2-(oxo-x0) ethyl]-13,13-bis[[3-[[2-(D-altronoylamino) ethyl]amino]-3-oxopropoxy]methyl]-6,9-bis[(acrboxy-x0)methyl]-11-(oxo-x0)-18-oxo-15-oxa-3,6,9,12,19-pentaazaheneicosanoato(3-)-x83,x80,x80,x0)]qua- (CA INDEX NAME)

PAGE 1-A

$$-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{NH}-\mathsf{C}-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{O}-\mathsf{CH}_2\\ \mathsf{NH}-\mathsf{C}-\mathsf{CH}_2-\mathsf{O}-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{C}-\mathsf{NH}-\mathsf{CH}_2-\mathsf{CH}_2\\ \mathsf{CH}_2-\mathsf{O}-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{C}-\mathsf{NH}-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{NH}-\mathsf{CH}_2\\ \mathsf{O}\\ \mathsf{O$$

PAGE 1-C

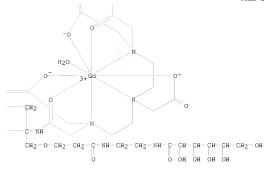


RN 1020213-19-7 CAPLUS
CN Gadolinium, aqua[6,9-bis[(carboxy-κ0)methyl]-21-(D-gluconoylamino)-3[2-[[2-[3-[[2-(D-gluconoylamino)ethyl]amino]-3-oxopropoxy]-1,1-bis[[3-[[2-(D-gluconoylamino)ethyl]amino]-2-(oxo-к0)ethyl]-13,13-bis[[3-[[2-(D-gluconoylamino)ethyl]amino]-3oxopropoxy]methyl]-11-(oxo-к0)-18-oxo-15-oxa-3,6,9,12,19pentaazaheneicosanoato(3-)-кN3,кN6,кN9,кO1]- (CA
INDEX NAME)

PAGE 1-B

$$-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{NH}-\mathsf{C}-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{O}-\mathsf{CH}_2\\ \mathsf{NH}-\mathsf{C}-\mathsf{CH}_2-\mathsf{O}-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{C}-\mathsf{NH}-\mathsf{CH}_2-\mathsf{CH}_2\\ \mathsf{CH}_2-\mathsf{O}-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{C}-\mathsf{NH}-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{NH}-\\ \mathsf{O} \\ \mathsf{O}$$

PAGE 2-A



RN 1020213-20-0 CAPLUS

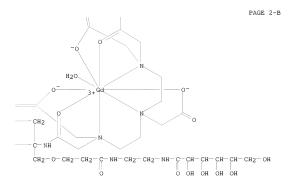
CN

 $\begin{array}{lll} {\rm Gadolinium,\ aqua[6,9-bis((carboxy-\kappa0))methyl]-2l-(D-mannonoylamino)-3-(2-[2-[3-[2-(D-mannonoylamino)=thyl]amino]-3-oxopropoxy]-1,1-bis[[3-[2-(D-mannonoylamino)=thyl]amino]-2-(oxo-\kappa0)ethyl]-13,13-bis[[3-[2-(D-mannonoylamino)=thyl]amino]-3-oxopropoxy[methyl]-11-(oxo-\kappa0)-18-oxo-15-oxa-3,6,9,12,19-pentaazahenelcosanoato(3-)-\kappa03,\kappa06,\kappa09,\kappa01]- \\ {\rm (CA} & {\rm CA} & {\rm CA}$ 

PAGE 1-A

$$- \, \operatorname{CH}_2 - \operatorname{CH}_2 - \operatorname{NH} - \operatorname{C} - \operatorname{CH}_2 - \operatorname{CH}_2 - \operatorname{O} - \operatorname{CH}_2 \\ - \operatorname{NH} - \operatorname{C} - \operatorname{CH}_2 - \operatorname{O} - \operatorname{CH}_2 - \operatorname{CH}_2 - \operatorname{C} - \operatorname{NH} - \operatorname{CH}_2 - \operatorname{CH}_2 - \operatorname{CH}_2 \\ - \operatorname{CH}_2 - \operatorname{O} - \operatorname{CH}_2 - \operatorname{CH}_2 - \operatorname{C} - \operatorname{NH} - \operatorname{CH}_2 - \operatorname{CH}_2 - \operatorname$$

PAGE 1-C

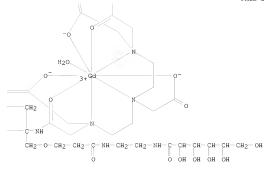


RN 1020213-21-1 CAPLUS
CN Gadolinium, aqua[6,9-bis[(carboxy-κ0)methyl]-21-(D-gulonoylamino)-3[2-[[2-[3-[[2-(D-gulonoylamino]ethyl]amino]-3-oxopropoxy]-1,1-bis[[3-[[2-(D-gulonoylamino)ethyl]amino]-3-oxopropoxy]methyl]-13,13-bis[[3-[[2-(D-gulonoylamino)ethyl]amino]-3oxopropoxy]methyl]-11-(oxo-к0)-18-oxo-15-oxa-3,6,9,12,19pent azazaheneicosanoato(3-)-кN3, кN6, кN9, кО1]- (CA
INDEX NAME)

PAGE 1-B

$$-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{NH}-\mathsf{C}-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{O}-\mathsf{CH}_2\\ \mathsf{NH}-\mathsf{C}-\mathsf{CH}_2-\mathsf{O}-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{C}-\mathsf{NH}-\mathsf{CH}_2-\mathsf{CH}_2\\ \mathsf{CH}_2-\mathsf{O}-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{C}-\mathsf{NH}-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{NH}-\\ \mathsf{O} \\ \mathsf{O}$$

PAGE 2-A



RN 1020213-22-2 CAPLUS

CN Gadolinium, aqua[6,9-bis[(carboxy-k0)methyl]-21-(D-idonoylamino)-3[2-[[2-[3-[[2-(D-idonoylamino)ethyl]amino]-3-oxopropoxy]-1,1-bis[[3-[[2-(D-idonoylamino)ethyl]amino]-3-oxopropoxy]methyl]ethyl]amino]-2-(oxok0)ethyl]-13,13-bis[[3-[[2-(D-idonoylamino)ethyl]amino]-3oxopropoxy]methyl]-11-(oxo-k0)-18-oxo-15-oxa-3,6,9,12,19pentaazaheneicosanoato(3-)-kN3,kN6,kN9,kO1]- (CA
INDEX NAME)

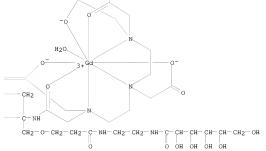
PAGE 1-A

$$- \, \operatorname{CH}_2 - \operatorname{CH}_2 - \operatorname{NH} - \operatorname{C} - \operatorname{CH}_2 - \operatorname{CH}_2 - \operatorname{O} - \operatorname{CH}_2 \\ - \operatorname{NH} - \operatorname{C} - \operatorname{CH}_2 - \operatorname{O} - \operatorname{CH}_2 - \operatorname{CH}_2 - \operatorname{C} - \operatorname{NH} - \operatorname{CH}_2 - \operatorname{CH}_2 - \operatorname{CH}_2 \\ - \operatorname{CH}_2 - \operatorname{O} - \operatorname{CH}_2 - \operatorname{CH}_2 - \operatorname{C} - \operatorname{NH} - \operatorname{CH}_2 - \operatorname{CH}_2 - \operatorname$$

PAGE 1-C

PAGE 2-B





RN 1020213-23-3 CAPLUS

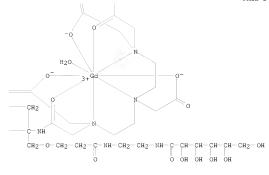
CN

Gadolinium, aqua[6,9-bis[(carboxy-k0)methyl]-21-(D-galactonoylamino)-3-[2-[[2-[3-[[2-(D-galactonoylamino)ethyl]amino]-3-oxopropoxy]-1,1-bis[[3-[[2-(D-galactonoylamino)ethyl]amino]-3-oxopropoxy]methyl]ethyl]amino]-2-(oxo-κO)ethyl]-13,13-bis[[3-[[2-(D-galactonoylamino)ethyl]amino]-3oxopropoxy]methyl]-11-(oxo-κ0)-18-oxo-15-oxa-3,6,9,12,19pentaazaheneicosanoato(3-)-KN3,KN6,KN9,KO1]- (CA INDEX NAME)

PAGE 1-B

$$-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{NH}-\mathsf{C}-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{O}-\mathsf{CH}_2\\ \mathsf{NH}-\mathsf{C}-\mathsf{CH}_2-\mathsf{O}-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{C}-\mathsf{NH}-\mathsf{CH}_2-\mathsf{CH}_2\\ \mathsf{CH}_2-\mathsf{O}-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{C}-\mathsf{NH}-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{NH}-\\ \mathsf{O} \\ \mathsf{O}$$

PAGE 2-A

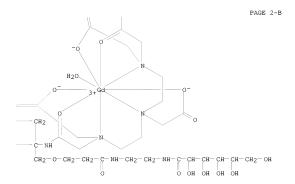


- RN 1020213-24-4 CAPLUS
- CN Gadolinium, aqua[6,9-bis[(carboxy-KO)methyl]-11-(oxo-KO)-18-oxo-3-[2-(oxo-KO)-2-[[2-3-oxo-3-[2-(D-talonoylamino)ethyl]amino]propoxy]-1,1-bis[(3-oxo-3-[2-(D-talonoylamino)ethyl]amino]propoxy]methyl]pethyl]amino]ethyl]amino]oxo-3-[[2-(D-talonoylamino)ethyl]amino]propoxy]methyl]-21-(D-talonoylamino)-15-oxa-3,6,9,12,19-pentaazaheneicosanoato(3-)-KN3,KN6,KN9,KO]-(CA INDEX NAME)

PAGE 1-A

$$- \, \operatorname{CH}_2 - \operatorname{CH}_2 - \operatorname{NH} - \operatorname{C} - \operatorname{CH}_2 - \operatorname{CH}_2 - \operatorname{O} - \operatorname{CH}_2 \\ - \operatorname{NH} - \operatorname{C} - \operatorname{CH}_2 - \operatorname{O} - \operatorname{CH}_2 - \operatorname{CH}_2 - \operatorname{C} - \operatorname{NH} - \operatorname{CH}_2 - \operatorname{CH}_2 - \operatorname{CH}_2 \\ - \operatorname{CH}_2 - \operatorname{O} - \operatorname{CH}_2 - \operatorname{CH}_2 - \operatorname{C} - \operatorname{NH} - \operatorname{CH}_2 - \operatorname{CH}_2 - \operatorname{C$$

PAGE 1-C

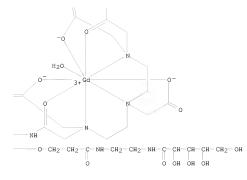


RN 1020213-25-5 CAPLUS

CN Gadolinium, aqua[21-(D-arabinonoylamino)-3-[2-[12-[3-[12-(D-arabinonoylamino) ethyl] amino]-3-oxopropoxy]-1,-bis[[3-[12-(D-arabinonoylamino) ethyl] amino]-3-oxopropoxy]methyl]ethyl]amino]-2-(oxo-KO) ethyl]-13,13-bis[[3-[12-(D-arabinonoylamino) ethyl]amino]-3-oxopropoxy]methyl]-6,9-bis[(carboxy-KO)methyl]-1]-(co-KO)-18-oxo-3-5,6,9,12,19-pentaazaheneicosanoato(3-)-KN3,KN6,KN9,KO]-(CA INDEX NAME)

PAGE 1-B

PAGE 2-A

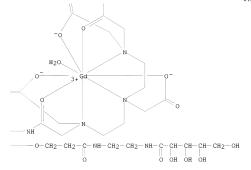


- RN 1020213-26-6 CAPLUS
- CN Gadolinium, aqua[6,9-bis[(carboxy-KO)methyl]-11-(oxo-KO)-18oxo-3-[2-(oxo-KO)-2-[[2-]3-oxo-3-[[2-(Dxylonoylamino)ethyl]amino]propoxy]-1,1-bis[[3-oxo-3-[[2-(Dxylonoylamino)ethyl]amino]propoxy]methyl]pethyl]amino]ethyl]-13,13-bis[[3oxo-3-[[2-(D-xylonoylamino)ethyl]amino]propoxy]methyl]-21-(Dxylonoylamino)-15-oxa-3,6,9,12,19-pentaazaheneicosanoato(3-)kN3,KN6,KN9,KO]- (CA INDEX NAME)

PAGE 1-A

PAGE 1-C

PAGE 2-B

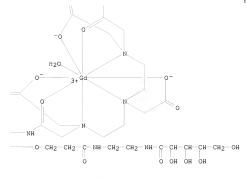


RN 1020213-27-7 CAPLUS

CN Gadolinium, aqua[6,9-bis[(carboxy-κ0)methyl]-21-(D-lyxonoylamino)-3[2-[[2-[3-[[2-(D-lyxonoylamino)ethyl]amino]-3-cxopropoxy]-1,1-bis[[3-[[2-(D-lyxonoylamino)ethyl]amino]-3-cxopropoxy]methyl]ethyl]amino]-2-(oxoκ0)ethyl]-13,13-bis[[3-[[2-(D-lyxonoylamino)ethyl]amino]-3oxopropoxy]methyl]-11-(oxo-κ0)-18-oxo-15-oxa-3,6,9,12,19pentaazaheneicosanoato(3-)-κN3,κN6,κN9,κOl]- (CA
INDEX NAME)

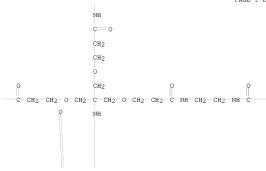
PAGE 1-B

PAGE 2-A



- RN 1020213-29-9 CAPLUS
- No. 1020x10-23-3 CAPLOO 3. TO PLOO 3. TO PL

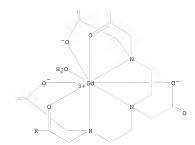
## PAGE 2-A



PAGE 2-C

0==

PAGE 3-B



PAGE 4-A

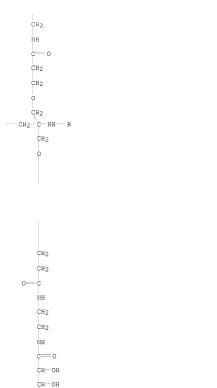
НО---

но\_\_

но-сн2-

PAGE 5-A

PAGE 6-B



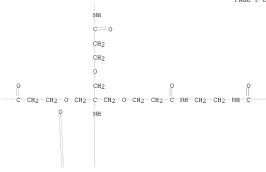
но

PAGE 7-B

RN 1020213-30-2 CAPLUS

CN Gadolinium, aqua[6,9-bis[(carboxy-κ0)methyl]-21-[(4-O-β-D-galactopyranosyl-D-gluconoyl)amino]-3-[2-[[2-1]-[2-[(4-O-β-D-galactopyranosyl-D-gluconoyl)amino]-3-oxopropoxy]-1,1-bis[[3-[[2-[(4-O-β-D-β-D-galactopyranosyl-D-gluconoyl)amino]+thyl]amino]-3-oxopropoxylmethyl]ethyl]amino]-2-(oxo-k0)ethyl]-11,1,13-bis[[3-[[2-[(4-O-β-D-galactopyranosyl-D-gluconoyl)amino]ethyl]amino]-3-oxopropoxylmethyl]-11-(oxo-K0)-18-0x-01-5-oxa-3,6,9,12,19-pentaazaheneicosanoato(3-)-κN3,κN6,κN9,κO1]- (CA

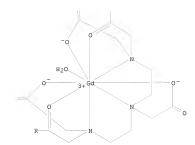
## PAGE 2-A



PAGE 2-C

0==

PAGE 3-B



PAGE 4-A

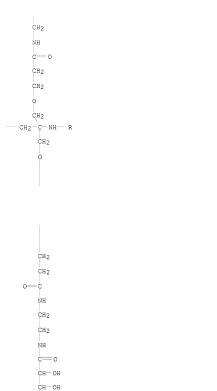
НО---

но\_\_

но-сн2-

PAGE 5-A

PAGE 6-B



но----

PAGE 7-B

IT 1020112-70-2P

DTPA

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of monosaccharide- and oligosaccharide-containing gadolinium

compds. and contrast media containing them for MRI)

RN 1020112-70-2 CAPLUS CN D-Allonamide, N,N'-[9-amino-4,14-dioxo-9-[[3-oxo-3-[[2-[(2,3,4,5,6-penta-0-

acetyl-D-allonoyl) aminojethyljaminojpropoxyjmethylj-7,11-dioxa-3,15-diazaheptadecane-1,17-dyljbie-, 2,2',3,3',4,4',5,5',6,6'-decaacetate (CA INDEX NAME)

#### Absolute stereochemistry.

OAc OAc

# RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L13 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
- TI Toward Iron Sensors: Bioinspired Tripods Based on Fluorescent Phenol-oxazoline Coordination Sites
- AB In the quest for fast throughput metal biosensors, it would be of interest to prepare fluorophoric ligands with surface-adhesive moieties. Biomimetic analogs to microbial siderophores possessing such ligands offer attractive model compds. and new opportunities to meet this challenge. The design, synthesis, and physicochem. characterization of biomimetic analogs of microbial siderophores from Paracoccus denitrificans and from the Vibrio genus are described. The (4S,5S)-2-(2-hydroxyphenyl)-5-methyl-4,5-dihydro-1,3-oxazole-4-carbonyl group (La), noted here as an HPO unit, was selected for its potential dual properties, serving as a selective iron(III) binder and simultaneously as a fluorophore. Three tripodal sym. analogs cis-Lb, cis-Lc, and trans-Lc, which mainly differ in the length of the spacers between the central carbon anchor and the ligating sites, were synthesized. These ferric-carriers were built from a tetrahedral carbon as an anchor, sym. extended by three converging iron-binding chains, each bearing a terminal HPO. The fourth chain could contain a surface-adhesive function (Lc). A combination of absorption and emission spectrophotometry, potentiometry, electrospray mass spectrometry, and electrochem, was used to fully characterize the corresponding ferric complexes and to determine their stability. The quenching mechanism is consistent with an intramol, static process and is more efficient for the analog with longer arms. Detection limits in the low nanogram per mL range, comparable with the best chemosensors based on natural peptide siderophores, have been determined These results clearly demonstrate that these tris(phenol-oxazoline) ligands in a tripodal arrangement firmly bind iron(III). Due to their fluorescent properties, the coordination event can be easily monitored, while the fourth arm is available for surface-adhesive moieties. The tripodal system is therefore an ideal candidate for integration with solid-state materials for the development of chip-based devices and anal. methodologies.
- AN 2007:216788 CAPLUS <<LOGINID::20080731>>
- DN 146:457805
- TI Toward Iron Sensors: Bioinspired Tripods Based on Fluorescent
- Phenol-oxazoline Coordination Sites
- AU Kikkeri, Raghavendra; Traboulsi, Hassan; Humbert, Nicolas; Gumienna-Kontecka, Elzbieta; Arad-Yellin, Rina; Melman, Galina; Elhabiri, Mourad; Albrecht-Gary, Anne-Marie; Shanzer, Abraham
- CS Department of Organic Chemistry, The Weizmann Institute of Science, Rehovot, Israel
- SO Inorganic Chemistry (Washington, DC, United States) (2007), 46(7), 2485-2497

CODEN: INOCAJ; ISSN: 0020-1669

PB American Chemical Society

DT Journal LA English

OS CASREACT 146:457805

IT 934995-49-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(bioinspired tripods based on fluorescent phenol-oxazoline coordination sites as iron sensors)

RN 934995-49-0 CAPLUS

CN 4,8-Dioxa-12,15,18-triazanonadecanamide, 6-ethyl-17-[(1R)-1-hydroxyethyl]-6-[(1R)-11-[(1R)-1-hydroxyethyl]-5,10,13-trioxo-2-oxa-6,9,12-triazatridec-1-yl]-N-[2-[([2S,3R)-3-hydroxy-1-oxo-2-[[2-(phenylmethoxy)benzoyl]amino]butyl]amino]ethyl]-11,16,19-trioxo-19-[2-(phenylmethoxy)phenyl]-, (17S)-(CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

#### RE.CNT 136 THERE ARE 136 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L13 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
- Solution phase biopolymer synthesis of oligodeoxyribonucleotides using TΙ multifunctional liquid phase carriers
- AB Multifunctional liquid phase carriers (LPCs) and methods of using LPCs for
- the preparation of biopolymers are provided. The LPCs are highly sym. compds.

that possess more than two points of attachment for biopolymer synthesis. The LPCs have the formula Sp(X1)n, where Sp is a highly sym. moiety such

that all X1 groups are equivalent X1 is a functional group that is suitable for biopolymer synthesis, including OH, SH, NH2, COOH and the like.

Biopolymers that may be produced using the methods provided include

oligonucleotides, peptides, protein nucleic acids (PNAs) and

KIND DATE

oligosaccharides. Analogs of the biopolymers may also be prepared using the methods. Thus decamer d(GACCGGCAGT) was prepared using multifunctional liquid phase carriers.

ADDITIONATION NO.

DATE

- AN 1999:708779 CAPLUS <<LOGINID::20080731>>
- DN 131:351620
- ΤI Solution phase biopolymer synthesis of oligodeoxyribonucleotides using multifunctional liquid phase carriers
- TN Koster, Hubert; Worl, Ralf
- PA USA
- SO PCT Int. Appl., 88 pp.
- CODEN: PIXXD2
- Patent DT
- LA English
- FAN.CNT 1 D3 MD31M 310

	PATENT NO.							DATE			APPLICATION NO.								
PI	WO					A2		19991104		WO 1999-US8939									
		W:	AE,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CU,	CZ,	
			DE,	DK,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	
			JP,	KE,	KG,	ΚP,	KR,	KZ,	LC,	LR,	LS,	LT,	LU,	LV,	MD,	MG,	MK,	MN,	
			MW,	MX,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	
			TR,	TT,	UA,	UG,	UZ,	VN,	YU,	ZA,	zw								
		RW:	GH,	GM,	KE,	LS,	MW,	SD,	SL,	SZ,	UG,	ZW,	ΑT,	BE,	CH,	CY,	DE,	DK,	
			ES,	FI,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	
								ML,											
											US 1998-67337					19980427			
	US 7094943																		
		AU 9936643																	
	EP	EP 1073668																	
		R:						ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,	
						LV,													
		US 20020007048									US 2000-484484			20000118					
	US 7038103																		
PRA:			98-67337																
		WO 1999-US8939							0426										

221898-81-3P 221898-82-4P RL: SPN (Synthetic preparation); PREP (Preparation)

(solution phase biopolymer synthesis of oligodeoxyribonucleotides using multifunctional liquid phase carriers)

RN 221898-81-3 CAPLUS

CN Thymidine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-, 3',3'''-[14,14-[[3-[[2-[(3-carboxy-1-oxopropy1)amino]ethy1]amino]-3-oxopropoxy]methy1]-4,9,19,24-tetraoxo-12,16-dioxa-5,8,20,23-tetraazaheptacosanedioate], 3',3'''-diester with 5'-0-[bis(4-methoxyphenyl)phenylmethyl]thymidine (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

PAGE 2-C

RN

221898-82-4 CAPLUS
Thymidine, 3',3'''-[14,14-[[3-[[2-[(3-carboxy-1-cxopropy1)amino]+thyl]amino]-3-oxopropoxy]methyl]-4,9,19,24-tetraoxo-12,16-dioxa-5,6,20,23-tetraozaheptacosanedioate], 3',3'''-diester with thymidine CN (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 2-B

ÓН

- L13 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN TI Synthesis of new liquid phase carriers for use in large scale oligodeoxyribonucleotide synthesis in solution
- GI

$$\begin{array}{c} {\rm CO-NH-CH_2-CH_2-NH_2} \\ \\ {\rm H_2N-CH_2-CH_2-NH-CO} \end{array} \\ \begin{array}{c} {\rm CO-NH-CH_2-CH_2-NH_2} \\ \end{array} \\ {\rm II} \end{array}$$

- AB The synthesis of multifunctional sym. primary amines, e.g. I, and the covalent binding of 5'-O-dimethoxytrityl-deoxynucleoside derivs, to their amino groups is described. Different strategies for dedimethoxytritylation including the use of strong acidic ion exchangers or protic acids and modified silica gels and/or gel permeation chromatog. are developed. The resulting liquid phase carriers are suitable for large scale oligodeoxyribonucleotide synthesis in solution using phosphoramidites and gel permeation chromatog, for fast isolation of intermediates.
- AN 1999:176579 CAPLUS <<LOGINID::20080731>>
- DN 130:267701
- ΤI Synthesis of new liquid phase carriers for use in large scale oligodeoxyribonucleotide synthesis in solution
- AII Worl, Ralf; Koster, Hubert
- CS Faculty of Chemistry, Department of Biochemistry and Molecular Biology, University of Hamburg, Hamburg, D-20146, Germany
- Tetrahedron (1999), 55(10), 2941-2956 SO CODEN: TETRAB; ISSN: 0040-4020
- PΒ Elsevier Science Ltd.
- DT Journal
- LA English
- TT 221898-81-3P
  - RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
    - (synthesis of new liquid phase carriers for use in large scale oligodeoxyribonucleotide synthesis in solution)
  - 221898-81-3 CAPLUS
- RN CN Thymidine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-, 3',3'''-[14,14-[[3-[[2-[(3-carboxy-1-oxopropy1)amino]ethy1]amino]-3-oxopropoxy]methy1]-
  - 4,9,19,24-tetraoxo-12,16-dioxa-5,8,20,23-tetraazaheptacosanedioate], 3',3'''-diester with 5'-0-[bis(4-methoxyphenyl)phenylmethyl]thymidine (9CI) (CA INDEX NAME)

Absolute stereochemistry.

\_\_ Me

MeO-

PAGE 1-C

### PAGE 2-B

#### PAGE 2-C

### 221898-82-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis of new liquid phase carriers for use in large scale oligodeoxyribonucleotide synthesis in solution)

- RN 221898-82-4 CAPLUS
- CN Thymidine, 3',3''-[14,14-[[3-[[2-[(3-carboxy-1-oxopropy1)amino]ethy1]amino]-3-oxopropoxy]methy1]-4,9,19,24-tetraoxo-12,16-dioxa-5,8,20,23-tetraazaheptacosanedioate], 3',3'''-diester with thymidine (9CI) (CA INDEX NAME)

Absolute stereochemistry.

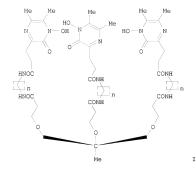
PAGE 1-A

PAGE 1-B

PAGE 2-B

# RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L13 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
- II N-hydroxyamide-containing heterocycles. Part 5. Synthesis of novel hexadentate ligands composed of N-hydroxy-2(IH)-pyrazinone, aliphatic diamine, and 1,1,1-tris(carboxyethoxymethyl)ethane, and properties of their ferric complexes



AB Novel hexadentate ligands I (n = 2, 4, 5, 6), containing N-hydroxy-2(1H)pyrazinone connected to tricarboxylic acid by an aliphatic diamine through amide bonds were synthesized. UV-visible spectra of the 1:1 M mixts. of I and ferric ion in aqueous solution and the mole ratio plot strongly supported the

formation of intramol. 1:1 ferric complexes. The relative stability consts. (log K 20.6-21.7) of the complexes were affected by the spacer length in a mol. Further, I showed higher Fe removal efficiency toward human transferrin than naturally occurring siderophore, desferrioxamine B. AN 1995:956600 CAPLUS <<LOGINID::20080731>>

DN 124:157320

OREF 124:29003a

- TΙ N-hydroxyamide-containing heterocycles. Part 5. Synthesis of novel hexadentate ligands composed of N-hydroxy-2(1H)-pyrazinone, aliphatic diamine, and 1,1,1-tris(carboxyethoxymethyl)ethane, and properties of their ferric complexes
- AII Ohkanda, Junko; Katoh, Akira
- CS Dep. Industrial Chem., Seikei Univ., Musashino, 180, Japan SO
- Tetrahedron (1995), 51(47), 12995-3002
- CODEN: TETRAB: ISSN: 0040-4020
- PB Elsevier
- DT Journal
- LA English
- ΙT 173414-90-9P
  - RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(for preparation of tris((((hydroxydimethyloxodihydropyrazyl)propanamide)alk ylaminocarbonyl)ethyloxymethyl)ethanes)

173414-90-9 CAPLUS RN

Pyrazinepropanamide, N,N'-[9-[[3-[[2-[[3-[3,4-dihydro-5,6-dimethyl-3-oxo-4-CN (phenylmethoxy)pyrazinyl]-1-oxopropyl]amino]ethyl]amino]-3oxopropoxy]methyl]-9-methyl-4,14-dioxo-7,11-dioxa-3,15-diazaheptadecane1,17-diyl]bis[3,4-dihydro-5,6-dimethyl-3-oxo-4-(phenylmethoxy)- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

PAGE 1-C

IT 173414-94-3P

CN

RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (USEs)

(preparation and complexation with iron and removal for iron from human transferrin)

RN 173414-94-3 CAPLUS

Pyrazinepropanamide, N,N'-[9-[[3-[[3-[3,4-dihydro-4-hydroxy-5,6-dimethyl-3-oxopyrazinyl)-1-oxopropyl]amino]ethyl]amino]-3-oxopyropxy]methyl]-9-methyl-4,14-dioxo-7,11-dioxa-3,15-diazaheptadecane-1,17-diyl]bis[3,4-dihydro-4-hydroxy-5,6-dimethyl-3-oxo-(9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{HO} \\ \text{NO} \\ \text{NO} \\ \text{NO} \\ \text{NO} \\ \text{CH}_2 - \text{CH}_2 -$$

$$-\operatorname{CH}_2-\operatorname{O-CH}_2-\operatorname{CH}_2-\operatorname$$

PAGE 2-B

=> d his

(FILE 'HOME' ENTERED AT 12:38:22 ON 31 JUL 2008)

FILE 'REGISTRY' ENTERED AT 12:38:29 ON 31 JUL 2008 L1 STRUCTURE UPLOADED

L2 1 S L1 L3 45 S L1 SSS FULL

FILE 'HCAPLUS' ENTERED AT 12:39:49 ON 31 JUL 2008

L4 41 S L3 L5 275759 S CONJUGAT? OR LINKER L6 10 S L4 AND L5

FILE 'REGISTRY' ENTERED AT 13:22:47 ON 31 JUL 2008

L7 STRUCTURE UPLOADED
L8 STRUCTURE UPLOADED
L9 STRUCTURE UPLOADED
L10 STRUCTURE UPLOADED
L11 1 S L10
L12 22 S L10 SSS FULL

FILE 'CAPLUS' ENTERED AT 13:52:40 ON 31 JUL 2008 L13 5 S L12

=> log hold

COST IN U.S. DOLLARS

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

SINCE FILE
TOTAL
ENTRY
ENTRY
SESSION
-4.00
-12.00
-12.00

SESSION WILL BE HELD FOR 120 MINUTES STN INTERNATIONAL SESSION SUSPENDED AT 13:52:59 ON 31 JUL 2008

Connecting via Winsock to STN

Welcome to STN International! Enter x:X

LOGINID:SSPTAEX01623

PASSWORD:

\* \* \* \* \* \* RECONNECTED TO SIN INTERNATIONAL \* \* \* \* \* \* SESSION RESUMED IN FILE 'CAPLUS' AT 14:00:50 ON 31 JUL 2008 FILE 'CAPLUS' ENTERED AT 14:00:50 ON 31 JUL 2008

COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 27.73 419.67 SINCE FILE TOTAL DISCOUNT AMOUNTS (FOR OUALIFYING ACCOUNTS) SESSION ENTRY CA SUBSCRIBER PRICE -4.00-12.00=> file registry COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 28.69 420.63 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE -4.00 -12.00

FILE 'REGISTRY' ENTERED AT 14:02:04 ON 31 JUL 2008

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the  ${\tt ZIC/VINITI}$  data file provided by InfoChem.

STRUCTURE FILE UPDATES: 30 JUL 2008 HIGHEST RN 1037244-07-7
DICTIONARY FILE UPDATES: 30 JUL 2008 HIGHEST RN 1037244-07-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when conducting  ${\tt SmartSELECT}$  searches.

REGISTRY includes numerically searchable data for experimental and precisted properties as well as relational distingtion and reperimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>

Uploading C:\Program Files\STNEXP\Queries\10780447linker2.str

chain nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 chain bonds:

exact/norm bonds :

```
exact bonds: 1-2 1-38 3-4 3-37 5-6 5-37 7-13 7-35 8-15 8-36 9-17 9-31 13-14 14-21 15-16 16-20 17-18 18-19 19-32 20-33 21-34 22-30 23-29 24-28 37-44 38-43 41-42 43-44
```

```
    Match level:
    1:CLASS | :CLASS | :CLA
```

#### L14 STRUCTURE UPLOADED

=> d 114 L14 HAS NO ANSWERS L14 STR

Structure attributes must be viewed using STN Express query preparation.

```
=> s 114
SAMPLE SEARCH INITIATED 14:02:29 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 35 TO ITERATE
```

100.0% PROCESSED 35 ITERATIONS 0 ANSWERS SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\* BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 346 TO 1054
PROJECTED ANSWERS: 0 TO 0

L15 0 SEA SSS SAM L14

=> s 114 sss full FULL SEARCH INITIATED 14:02:34 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 682 TO ITERATE

100.0% PROCESSED 682 ITERATIONS SEARCH TIME: 00.00.01

L16 0 SEA SSS FUL L14